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Quasiclassical Analysis of the Three-dimensional Schrödinger's Equation and Its Solution

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Abstract

The three-dimensional Schrödinger's equation is analyzed with the help of the correspondence principle between classical and quantum-mechanical quantities. Separation is performed after reduction of the original equation to the form of the classical Hamilton-Jacobi equation. Each one-dimensional equation obtained after separation is solved by the conventional WKB method. Quasiclassical solution of the angular equation results in the integral of motion $\vec{M}^2 = (l+\frac{1}{2})^2\hbar^2$ and the existence of nontrivial solution for the angular quantum number $l = 0$. Generalization of the WKB method for multi-turning-point problems is given. Exact eigenvalues for solvable and some "insoluble" spherically symmetric potentials are obtained. Quasiclassical eigenfunctions are written in terms of elementary functions in the form of a standing wave.

1. Introduction

Basic equation of quantum mechanics, the Schrödinger's wave equation, is usually solved in terms of special functions or numerically; for several potentials, the equation is solved exactly [1]. The general approach to solve the Schrödinger's equation for the solvable potentials[1] is to reduce this equation to the equation for hypergeometric function or some special function. To do that one needs to find first a special transformation for the wave function and its arguments to reduce the original equation to the hypergeometric form. After that using certain requirements (defined by boundary conditions) to the hypergeometric function one can write the corresponding solution for the problem under consideration, i.e. the eigenfunctions and the corresponding eigenvalues.

This is rather a mathematical approach to solve the eigenvalue problem in quantum mechanics; the corresponding methods and solutions of the wave equation for some potentials have been developed long before the creation of quantum mechanics. There are several features of this exact mathematical method that should be clarified from the physical point of view. One of them is related to the S-wave state. The radial Schrödinger's equation has no the centrifugal term for the orbital quantum number $l = 0$. From the physical point of view, this means that the problem does not have the left turning point. In order for the physical system to have a stable bound state (discrete spectrum) two turning points are required (see Ref. [1], for instance). However, solving the radial wave

[1]By "solvable" potentials we mean those models for which the eigenvalue problem can be reduced to a hypergeometric function by a suitable transformation.

equation for $l > 0$, one obtains energy eigenvalues for all l including $l = 0$. Another feature is related to the angular dependence. The angular eigenfunction for the ground state, $Y_{00}(\theta, \varphi) = const$, i.e. no nontrivial solution exists. Meanwhile, as in the case of radial dependence, it might be a function with no zeroes of the type of a standing half-wave.

There is another approach to the eigenvalue problem in quantum mechanics. This is the quasiclassical method which is well known and widely used mainly as the Wentzel-Kramers-Brillouin (WKB) approximation [2]-[4] applicable in the case when the de Broglie wavelength, $\lambda = h/p$ ($h = 2\pi\hbar$), is changing slowly. In several cases of interest, the WKB method yields the exact energy levels, however, its correct application results in the exact energy eigenvalues for *all* known solvable potentials.

The quasiclassical method is based on the correspondence principle between classical functions and operators of quantum mechanics. The correspondence principle is used to derive the wave equation in quantum mechanics. In Ref. [5] this principle has been used to derive the semiclassical wave equation appropriate in the quasiclassical region. It was shown that the standard WKB method (to leading order in $\hbar$) is the appropriate method to solve this equation.

In this work we solve the multi-dimensional Schrödinger's equation by the quasiclassical method. Unlike known approaches, instead of modification of one-dimensional equations obtained after separation, we analyze an original multi-dimensional Schrödinger's equation and reduce it to the equation in canonical form (without first derivatives). Separation is performed after reduction of the equation obtained to the form of the classical Hamilton-Jacobi equation. We show that the main question of the exactness of the quasiclassical method is tightly connected with the correspondence principle, i.e. the form of the generalized moments obtained after separation of the wave equation; the moments obtained after separation have to coincide with the corresponding classic generalized moments. The quantization condition is written with help of the argument's principle in the complex plane that allows us to generalize the quasiclassical method for multi-turning-point problems and obtain the exact energy eigenvalues for all known solvable potentials and, also, for some "insoluble" problems with more then two turning points.

The quasiclassical method reproduces not only the exact energy spectrum for known potentials but has new important features. One of the consequences of the quasiclassical solution of the multi-dimensional Schrödinger's equation is the existence of a nontrivial angular solution at $l = 0$, $\tilde{Y}_{00}^{WKB}(\theta, \varphi)$, which describes the quantum fluctuations of the angular moment. This method allows us to show apparently the contribution of quantum fluctuations of the angular momentum into the energy of the ground state.

2. Exactness of the WKB method

It is well known that the exact eigenvalues can be defined with the help of the asymptotic solution, i.e. the exact solution and its asymptote correspond to the same exact eigenvalue of the problem under consideration. The asymptotic solutions in quantum mechanics can be obtained by the WKB method. Therefore the quasiclassical method should reproduce the exact energy spectrum.

Intriguing results have been obtained with the help of the supersymmetric WKB method (SWKB) [6]-[8], which is a modification of the standard WKB quantization for ob-

taining the quasiclassical eigenvalues of nonrelativistic Hamiltonians. It was demonstrated that the leading-order SWKB quantization condition in each and every case reproduces the exact energy eigenvalues for a class of solvable potentials. For these models, solutions can be written in terms of elementary functions.

Successes of the SWKB quantization rule have revived interest in the original WKB quantization condition. In several common applications the method gives very accurate results. Proofs of varying degrees of rigor have been advanced that demonstrate the exactness of the standard WKB quantization condition [2],[6]-[14]. The existing proofs of exactness of the WKB approximation are not entirely rigorous since the correction terms are only asymptotically valid, i.e., as $\hbar \to 0$ [10]. Furthermore, in the cases when a modified WKB integral gives the exact eigenvalues, it is not even clear which "correction" must be shown to be zero.

The standard lowest-order WKB prescription reproduces the exact energy levels for the harmonic oscillator in the Cartesian coordinates x, y, and z. But just this problem is correctly formulated in the framework of the quasiclassical approach; in the Cartesian coordinates, the Schrödinger's equation has the required canonical form and the generalized moments for each degree of freedom coincide with the corresponding classic moments. As for other coordinate systems, for example spherical, the WKB method does not reproduce the exact energy levels unless one supplements it with Langer-like correction terms.

For the central potential $V(r)$, the Schrödinger's equation can be written in the spherical coordinates as

$$(-i\hbar)^2 \left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\,\theta}\frac{\partial}{\partial\theta}\left(\sin\,\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\psi(\vec{r}) = 2m[E - V(r)]\psi(\vec{r}). \tag{1}$$

The standard solution of this equation is the following. If one substitutes $\psi(\vec{r}) = [U(r)/r]$ $[\Theta(\theta)/\sqrt{\sin\theta}]\Phi(\varphi)$ into Eq. (1), one obtains (after separation) the following three reduced one-dimensional equations

$$\left[\hbar^2\frac{d^2}{dr^2} + 2m(E - V) - \frac{\vec{L}^2}{r^2}\right]U(r) = 0, \tag{2}$$

$$\left(\hbar^2\frac{d^2}{d\theta^2} + \vec{L}^2 + \frac{\hbar^2}{4} - \frac{L_z^2 - \frac{\hbar^2}{4}}{\sin^2\theta}\right)\Theta(\theta) = 0, \tag{3}$$

$$\left(\hbar^2\frac{d^2}{d\varphi^2} + L_z^2\right)\Phi(\varphi) = 0. \tag{4}$$

Exact solution of Eq. (3) gives, for the squared angular momentum $\vec{L}^2$, $\vec{L}^2 = l(l+1)\hbar^2$. Application of the leading-order WKB quantization condition [1],

$$\int_{x_1}^{x_2}\sqrt{p^2(x,E)}dx = \pi\hbar\left(n + \frac{1}{2}\right), \qquad n = 0,\, 1,\, 2,\, ..., \tag{5}$$

to the radial Eq. (2) does not reproduce the exact energy spectrum {here in (5) x_1 and x_2 are the classic turning points and $p^2(x,E) = 2m[E - V(x)]$}. The problem comes from the form of the centrifugal term, $l(l+1)\hbar^2/r^2$.

To overcome this problem in particular case of the Coulomb potential, a special techniques has been developed. In order for the first-order WKB approximation to give the exact eigenvalues, the quantity $l(l+1)$ in Eq. (2) must be replaced by $(l+\frac{1}{2})^2$ [11]. The reason for this modification (for the special case of the Coulomb potential) was pointed out by Langer (1937) [11] from the Langer transformation $r = e^x$, $U(r) = e^{x/2}X(x)$. However, for other spherically symmetric potentials, in order to obtain the appropriate Langer-like correction terms, another special transformation of the wave function (w.f.) and its arguments is required.

There are several other related problems in the semiclassical consideration of the radial Schrödinger equation (2). (i) The WKB solution of the radial equation is irregular at $r \to 0$, i.e. $R^{WKB}(r) \propto r^{\lambda}/\sqrt{r}$, $\lambda = \sqrt{l(l+1)}$, whereas the exact solution in this limit is $R(r) \propto r^l$. (ii) Equation (2) has no the centrifugal term when $l = 0$, i.e. the radial problem has only one turning point and one can not use the WKB quantization condition (5) derived for two-turning-point problems. However, solving the equation for $l > 0$ by known exact methods one obtains energy eigenvalues for all l. (iii) The WKB solution of equation (3) has analogous to the radial one, incorrect behavior at $\theta \to 0$: $\Theta^{WKB}(\theta) \propto \theta^{\mu}$, $\mu^2 = m^2 - \hbar^2/4$, while the exact regular solution in this limit is $\Theta_l^m(\theta) \propto \theta^{|m|}$. Angular eigenfunction $Y_{00}(\theta,\varphi) = const$, i.e. no nontrivial solution exists.

As practical use shows the standard leading-order WKB approximation *always* reproduces the exact spectrum for the solvable spherically symmetric potentials $V(r)$ if the centrifugal term in the radial Schrödinger's equation has the form $(l+\frac{1}{2})^2\hbar^2/r^2$. As will be shown below the centrifugal term of such a form can be obtained from the WKB solution of equation (1) if separation of this three-dimensional equation has performed with the help of the correspondence principle.

3. Separation of the Schrödinger's equation

There are two essential features of the WKB method. First, the method was developed to solve the Schrödinger's equation in canonical form (without first derivatives). Second, in the quasiclassical method, the classic quantities such as classic momentum, classic action, phase, etc., are used. (For example, in the WKB quantization condition, the classic generalized momentum in the phase-space integral is used). For the harmonic oscillator in the Cartesian coordinates, the generalized moments in the original equation and moments obtained after separation coincide with the corresponding classic moments. Just for this problem, the standard WKB method (in one and multi-dimensional cases) reproduces the exact energy levels without any additional correction terms.

The generalized moments in Eqs. (2)-(4) obtained from separation of Eq. (1) are different from the corresponding classic moments. As a result, the WKB method does not reproduce the exact energy levels for the spherically symmetric potentials (unless one supplements it with Langer-like correction terms). The reason is the form of the squared angular momentum, $\vec{L}^2 = l(l+1)\hbar^2$, which is obtained from solution of the equation

(3). In the WKB method, in order to reproduce the exact energy spectrum, the term $(l+\frac{1}{2})^2\hbar^2$ should be used in the centrifugal term. This term, $M^2=\vec{L}^2+\hbar/4$, is in the angular equation (3), but is not in the radial equation (2).

Let us show that the term $(l+\frac{1}{2})^2\hbar^2$ can be obtained from the quasiclassical solution of the reduced Schrödinger's equation. For this, exclude in Eq. (1) the first derivatives that can be easily done with the help of the following operator identity:

$$\frac{d}{dx}g(x)\frac{d}{dx}\equiv\left[\sqrt{g(x)}\frac{d^2}{dx^2}-\frac{d^2}{dx^2}\sqrt{g(x)}\right]\sqrt{g(x)}. \tag{6}$$

Then, after dividing by $\tilde{\psi}(\vec{r})=\tilde{R}(r)\tilde{\Theta}(\theta)\tilde{\Phi}(\varphi)$, where $\tilde{R}(r)=rR(r)$, $\tilde{\Theta}(\theta)=\sqrt{\sin(\theta)}\Theta(\theta)$, $\tilde{\Phi}(\varphi)=\Phi(\varphi)$, we obtain the equation

$$-\hbar^2\frac{\tilde{R}''_{rr}}{\tilde{R}}+\frac{1}{r^2}\left(-\hbar^2\frac{\tilde{\Theta}''_{\theta\theta}}{\tilde{\Theta}}-\frac{\hbar^2}{4}\right)+\frac{1}{r^2\sin^2\theta}\left(-\hbar^2\frac{\tilde{\Phi}''_{\varphi\varphi}}{\tilde{\Phi}}-\frac{\hbar^2}{4}\right)= 2m[E-V(r)]. \tag{7}$$

Introducing the notations,

$$\left(\frac{\partial S_0}{\partial r}\right)^2=-\hbar^2\frac{\tilde{R}''_{rr}}{\tilde{R}}, \tag{8}$$

$$\left(\frac{\partial S_0}{\partial \theta}\right)^2=-\hbar^2\frac{\tilde{\Theta}''_{\theta\theta}}{\tilde{\Theta}}-\frac{\hbar^2}{4}, \tag{9}$$

$$\left(\frac{\partial S_0}{\partial \varphi}\right)^2=-\hbar^2\frac{\tilde{\Phi}''_{\varphi\varphi}}{\tilde{\Phi}}-\frac{\hbar^2}{4}, \tag{10}$$

we can write Eq. (7) in the form of the classic Hamilton-Jacobi equation,

$$\left(\frac{\partial S_0}{\partial r}\right)^2+\frac{1}{r^2}\left(\frac{\partial S_0}{\partial \theta}\right)^2+\frac{1}{r^2\sin^2\theta}\left(\frac{\partial S_0}{\partial \varphi}\right)^2=2m\left[E-V(r)\right], \tag{11}$$

where $S_0=S_0(\vec{r},E)$ is the classic action of the system.

Using the correspondence principle, we see, from Eq. (11), that Eqs. (8)-(10) are the squared generalized moments expressed via the quantum-mechanical quantities. Now, let us separate equation (11). Then, taking into account Eqs. (8)-(10), we obtain the following system of the second-order differential equations in canonical form

$$\left(-i\hbar\frac{d}{dr}\right)^2\tilde{R}=\left[2m(E-V)-\frac{\vec{M}^2}{r^2}\right]\tilde{R}, \tag{12}$$

$$\left[\left(-i\hbar\frac{d}{d\theta}\right)^2-\left(\frac{\hbar}{2}\right)^2\right]\tilde{\Theta}(\theta)=\left(\vec{M}^2-\frac{M_z^2}{\sin^2\theta}\right)\tilde{\Theta}(\theta), \tag{13}$$

$$\left[\left(-i\hbar\frac{d}{d\varphi}\right)^2-\left(\frac{\hbar}{2}\right)^2\right]\tilde{\Phi}(\varphi)=M_z^2\tilde{\Phi}(\varphi), \tag{14}$$

where $\vec{M}^2$ and M_z^2 are the constants of separation and, at the same time, integrals of motion.

Equations (12)-(14) have the quantum-mechanical form $\hat{f}\psi = f\psi$, where f is the physical quantity (the squared generalized momentum) and $\hat{f}$ is the corresponding operator. We see that the term $\hbar^2/4$ in the left-hand side of the equations is related to the squared angular momentum operator. This term disappears in the leading $\hbar$ approximation [5] and the equations (12)-(14) can be written in the general form as

$$\left(-i\hbar\frac{d}{dq}\right)^2 \psi(q) = [\lambda^2 - U(q)]\psi(q). \tag{15}$$

The squared generalized moments in the right-hand sides are the same as the classic ones. The use of these moments in the WKB quantization condition and WKB solution yields the exact energy spectra for the central-field potentials and does not result in the difficulties of the WKB method mentioned above.

4. Solution of the Schrödinger's equation

In this section we consider quasiclassical solution of the Schrödinger's equation for the spherically symmetric potentials. In order for the approach we consider here to be self-consistent we have to solve each equation obtained after separation by the same method, i.e. the WKB method. The quasiclassical method is general enough and the WKB formulas can be written differently, i.e. on the real axis [1] and in the complex plane [2]. Most general form of the WKB solution and quantization condition can be written in the complex plane.

The WKB quantization in the complex plane. The WKB method is usually used to solve one-dimensional two turning point problems. Within the framework of the WKB method the solvable potentials mean those potentials for which the eigenvalue problem has two turning points. However the WKB method can be used to solve problems with more then two turning points. In this case formulation in the complex plane is the most appropriate.

Consider Eqs. (12)-(14) in the framework of the quasiclassical method. Solution of each of these equations [in the general form Eq. (15)] we search in the form [2]

$$\psi_\lambda(z) = A\,\exp\left[\frac{i}{\hbar}S(z,\lambda)\right], \tag{16}$$

where A is the arbitrary constant. The function $S(z,\lambda)$ is written as the expansion in powers of $\hbar$, $S(z,\lambda) = S_0(z,\lambda) + \hbar S_1(z,\lambda) + \frac{1}{2}\hbar^2 S_2(z,\lambda) + \ldots$. In the leading $\hbar$ approximation the WKB solution of Eqs. (12)-(14) can be written in the form

$$\psi^{WKB}(z) = \frac{A}{\sqrt{p(z,\lambda)}}\exp\left[\pm\frac{i}{\hbar}\int_{z_0}^{z}\sqrt{p^2(z,\lambda)}dz\right]. \tag{17}$$

In quantum mechanics, quantum numbers are determined as number of zeroes of the w.f. in the physical region. In the complex plane, the number of zeroes N of a function

$y(z)$ inside the contour C is defined by the argument's principle [15, 16]. For the w.f. $\psi_\lambda(z)$, according to this principle we have

$$\oint_C \frac{\psi'_\lambda(z)}{\psi_\lambda(z)} dz = 2\pi i N, \tag{18}$$

where $\psi'_\lambda(z)$ is the derivative of the function $\psi_\lambda(z)$ over the variable z [see Ref. [17] for more information about the condition (18)]. Contour C is chosen such that it includes cuts (therefore, zeroes of the w.f.) between the turning points where $p^2(z,\lambda) = \lambda^2 - U(z) > 0$.

Substitution of Eq. (17) into (18) results in the quantization condition

$$\oint \sqrt{p^2(z,\lambda)} dz + i\frac{\hbar}{2} \oint \frac{p'(z,\lambda)}{p(z,\lambda)} dz = 2\pi\hbar N. \tag{19}$$

In the case, when $p(z,\lambda)$ is a smooth function of the spatial variable and the equation $\lambda^2 - U(z) = 0$ has two roots (turning points), the quantization condition (19) takes the form

$$\oint \sqrt{p^2(z,\lambda)} dz = 2\pi\hbar \left(N + \frac{1}{2}\right). \tag{20}$$

In particular, for $p^2(z,\lambda) = \lambda^2$, the quantization condition is

$$\oint \sqrt{p^2(z,\lambda)} dz = 2\pi\hbar N. \tag{21}$$

In the next section we solve the three-dimensional Schrödinger equation for several spherically symmetric potentials by the method under consideration.

A. The angular momentum eigenvalues. Equations (13) and (14) determine the squared angular momentum eigenvalues, $\vec{M}^2$, and its projection, M_z, respectively. The quantization condition (21) appropriate to the angular equation (14),

$$\oint M_z d\varphi = 2\pi\hbar m, \tag{22}$$

gives $M_z = \hbar m$, $m = 0, 1, 2, ...$ The corresponding quasiclassical solution is

$$\tilde{\Phi}_m(\varphi) = C_1\, e^{im\varphi} + C_2\, e^{-im\varphi}, \tag{23}$$

where C_1 and C_2 are the arbitrary constants.

The quantization condition (20) appropriate to Eq. (13) is

$$I = \oint_C \sqrt{\vec{M}^2 - \frac{M_z^2}{\sin^2\theta}} d\theta = 2\pi\hbar \left(n_\theta + \frac{1}{2}\right), \quad n_\theta = 0, 1, 2, ... \tag{24}$$

To calculate the integral (24) (as other hereafter) we use the method of stereographic projection. This means that, instead of integration about a contour C enclosing the classical turning points, we exclude the singularities outside the contour C, i.e., at $\theta = 0$ and ∞ in this particular case. Excluding these infinities we have, for the integral (24), $I = I_0 + I_\infty$. Integral $I_0 = -2\pi M_z$, and I_∞ is calculated with the help of the replacement

$z = e^{i\theta}$ that gives $I_\infty = 2\pi\sqrt{\vec{M}^2} \equiv 2\pi M$. Therefore, $I = 2\pi(M - M_z)$ and we obtain, for the squared angular momentum eigenvalues,

$$\vec{M}^2 = \left(l + \frac{1}{2}\right)^2 \hbar^2, \tag{25}$$

where $l = n_\theta + m$. Thus the quasiclassical solution of the Schrödinger's equation results in the squared angular momentum eigenvalues (25). This means the centrifugal term in the radial Eq. (12) has the form $(l + \frac{1}{2})^2\hbar^2/r^2$ for *all* spherically symmetric potentials.

As known the WKB solution $\Theta^{WKB}(\theta)$ of the equation (3) has incorrect asymptotes at $\theta \to 0$ and π. At the same time, the WKB solution of Eq. (13), which corresponds to the eigenvalues (25), has the correct asymptotic behavior at these points for all l. So far, as the generalized momentum $p(\theta) \simeq \frac{|m|}{\theta}$ at $\theta \to 0$, this gives, for the WKB solution in the representation of the wave function $\psi(\vec{r})$, $\Theta_l^m(\theta) = \tilde{\Theta}^{WKB}(\theta)/\sqrt{\sin\theta} \propto \theta^{|m|}$ which corresponds to the behavior of the known exact solution $Y_{lm}(\theta, \varphi)$ at $\theta \to 0$.

In the classically allowed region, where $p^2(\theta, M) = \vec{M}^2 - M_z^2/\sin^2\theta > 0$, the leading-order WKB solution of Eq. (13) is

$$\tilde{\Theta}^{WKB}(\theta) = \frac{B}{\sqrt{p(\theta, M)}} \cos\left[\int_{\theta_1}^{\theta} p(\theta, M)d\theta - \frac{\pi}{4}\right]. \tag{26}$$

The normalized quasiclassical solution far from the turning points, where $p(\theta, M) \simeq (l + \frac{1}{2})\hbar$, can be written in elementary functions as

$$\tilde{\Theta}_l^m(\theta) = \sqrt{\frac{2l+1}{\pi(l - m + \frac{1}{2})}} \cos\left[\left(l + \frac{1}{2}\right)\theta + \frac{\pi}{2}(l - m)\right], \tag{27}$$

where we have took into account that the phase-space integral at the classic turning point θ_1 is $\chi(\theta_1) = -\frac{\pi}{2}(n_\theta + \frac{1}{2})$ and $\chi(\theta_2) = \frac{\pi}{2}(n_\theta + \frac{1}{2})$ at $\theta = \theta_2$. We see that the eigenfunctions (27) are either symmetric or antisymmetric. The corresponding WKB solution, $\tilde{Y}_{lm}^{WKB}(\theta, \varphi) = \tilde{\Theta}_l^m(\theta)\tilde{\Phi}_m(\varphi)$, where the normalized eigenfunction $\tilde{\Phi}_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{\pm im\varphi}$, in the representation of the w.f. $\tilde{\psi}(\vec{r})$ is

$$\tilde{Y}_{lm}^{WKB}(\theta, \varphi) = \frac{1}{\pi}\sqrt{\frac{l + \frac{1}{2}}{l - m + \frac{1}{2}}} \cos\left[\left(l + \frac{1}{2}\right)\theta + \frac{\pi}{2}(l - m)\right] e^{\pm im\varphi}. \tag{28}$$

Remind some results concerning the semiclassical approach in quantum mechanics. The general form of the semiclassical description of quantum-mechanical systems have been considered in Ref. [18]. It was shown that the semiclassical description resulting from Weyl's association of operators to functions is identical with the quantum description and no information need to be lost in going from one to the another. What is more "the semiclassical description is more general than quantum mechanical description..." [18]. The semiclassical approach merely becomes a different representation of the same algebra as that of the quantum mechanical system, and then the expectation values, dispersions, and dynamics of both become identical.

One of the fundamental features of quantum mechanical systems is nonzero minimal energy which corresponds to quantum oscillations. The corresponding w.f. has no zeroes in the physical region. Typical example is the harmonic oscillator.

Eigenvalues of the one-dimensional harmonic oscillator are $E_n = \hbar\omega(n + \frac{1}{2})$, i.e. the energy of zeroth oscillations $E_0 = \frac{1}{2}\hbar\omega$. In three-dimensional case, in the Cartesian coordinates, the eigenvalues of the oscillator are $E_n = \hbar\omega(n_x + n_y + n_z + \frac{3}{2})$ [19], i.e. each degree of freedom contributes to the energy of the ground state, $E_0 = E_{0,x} + E_{0,y} + E_{0,z} = \frac{3}{2}\hbar\omega$. Energy of the ground state should not depend on coordinate system. This means that, in the spherical coordinates, each degree of freedom (radial and angular) should contribute to the energy of zeroth oscillations. In many applications and physical models a nonzero minimal angular momentum M_0 is introduced (phenomenologically) in order to obtain physically meaningful result (see, for instance, Ref. [20]). However, the existence of M_0 follows from the quasiclassical solution of Eq. (13) [5, 21].

Consider the WKB eigenfunction (28) for the ground state. Setting in (28) $m = 0$ and $l = 0$, we obtain the nontrivial solution in the form of a standing half-wave [remind that the spherical function $Y_{00}(\theta, \varphi) = const$],

$$\tilde{Y}_{00}^{WKB}(\theta, \varphi) = \frac{1}{\pi} \cos\frac{\theta}{2}. \tag{29}$$

The corresponding eigenvalue is

$$M_0 = \frac{\hbar}{2}. \tag{30}$$

The eigenvalue (30) contributes to the energy of zeroth oscillations. This means that (29) can be considered as solution, which describes the quantum fluctuations of the angular momentum. Note, that the eigenfunction of the ground state, $\tilde{Y}_{00}^{WKB}(\theta, \varphi)$, is symmetric. Below, we solve the radial equation (12) for some spherically symmetric potentials and show the contribution of the eigenvalue M_0 to the energy of the ground state.

B. The Coulomb problem $V(r) = -\frac{\alpha}{r}$. The WKB quantization condition (19) appropriate to the radial equation (2) with the Coulomb potential does not reproduce the exact energy levels unless one supplements it with Langer-like correction terms. Another problem is that the radial Schrödinger's equation (2) has no the centrifugal term at $l = 0$ and one can not use the WKB quantization condition (derived for two-turning-point problems) to calculate the energy of the ground state directly from this equation. We do not run into such a problem in case of Eqs. (12)-(14). As follows from the above consideration, the centrifugal term $(l + \frac{1}{2})^2\hbar^2/r^2$ is the same for all spherically symmetric potentials and the WKB method reproduces the exact energy spectrum for all l and n_r.

For the radial equation (12) with the Coulomb potential, the WKB quantization condition (20) is

$$I = \oint_C \sqrt{2mE + \frac{2m\alpha}{r} - \frac{\vec{M}^2}{r^2}}dr = 2\pi\hbar\left(n_r + \frac{1}{2}\right), \tag{31}$$

where the integral is taken about a contour C inclosing the turning points r_1 and r_2. Using the method of stereographic projection, we should exclude the singularities outside the

contour C, i.e. at $r = 0$ and ∞. Excluding these infinities we have, for the integral (31), $I = I_0 + I_\infty$, where $I_0 = 2\pi i\sqrt{-\vec{M}^2} \equiv -2\pi M$ and $I_\infty = 2\pi i\alpha m/\sqrt{2mE}$. The sequential simple calculations result in the exact energy spectrum

$$E_n = -\frac{\alpha^2 m}{2[(n_r + \frac{1}{2})\hbar + M]^2}. \tag{32}$$

For the energy of zeroth oscillations we have, from Eq. (32), $E_0 = -\frac{1}{2}\alpha^2 m(\frac{\hbar}{2} + M_0)^{-2}$, that apparently shows the contribution of the quantum fluctuations of the angular momentum (see Eq. (30)) into the energy of the ground state E_0 [21]. The radial quasiclassical eigenfunctions, $\tilde{R}_n^{WKB}(r)$, inside the classical region $[r_1, r_2]$ far from the turning points r_1 and r_2 are written in elementary functions in the form of a standing wave [5],

$$\tilde{R}_n(r) = A\cos\left(\frac{1}{\hbar}p_n r + \frac{\pi}{2}n_r\right), \tag{33}$$

where we have took into account that the phase-space integral (31) at the classic turning point r_1 is $\chi(r_1) = -\frac{\pi}{2}(n_r + \frac{1}{2})$. Here A is the normalization constant and p_n is the eigenmomentum expressed via the energy eigenvalue E_n, $p_n = \sqrt{2m|E_n|}$. The eigenfunctions (33) are either symmetric or antisymmetric.

C. The three-dimensional harmonic oscillator $V(r) = \frac{1}{2}m\omega^2 r^2$. The three-dimensional harmonic oscillator is another classic example of the exactly solvable problems in quantum mechanics. The problem has 4 turning points, r_1, r_2, r_3, and r_4, but only two of them, r_3 and r_4, lie in the physical region $r > 0$.

The problem is usually solved with the help of the replacement $x = r^2$ which reduces the problem to the 2-turning-point (2TP) one. But this problem can be solved as the 4TP problem in the complex plane. Because of importance of the oscillator potential in many applications and with the purpose of further development of the WKB method, we shall solve the problem by two methods, on the real axis as 2TP problem and then in the complex plane as 4TP problem.

Consider first the physical region $r > 0$, where the problem has two turning points. The leading-order WKB quantization condition (20) then is

$$I = \int_{r_3}^{r_4}\sqrt{2mE - (m\omega r)^2 - \frac{\vec{M}^2}{r^2}}dr = \pi\hbar\left(n_r + \frac{1}{2}\right), \tag{34}$$

where n_r is the number of zeroes of the w.f. between the classic turning points r_3 and r_4. Integral (34) is reduced to the above case of the Coulomb potential with the help of the replacement $z = r^2$. Integration result is $I = \pi(E/\omega - M)/2$ and we obtain, for the energy eigenvalues,

$$E_n = \omega\left[2\hbar\left(n_r + \frac{1}{2}\right) + M\right]. \tag{35}$$

So far, as $M = (l + \frac{1}{2})\hbar$, we obtain the exact energy spectrum for the isotropic oscillator. Energy of the ground state is $E_0 = \omega(\hbar + M_0)$, where M_0 is the contribution of quantum fluctuations of the angular momentum.

Emphasize the following in this solution. The 4TP problem has been solved as the 2TP problem; we have applied the 2TP quantization condition (20) to the 4TP problem that is not quite correct. We have obtained the correct result because the potential is symmetric and the replacement $x = r^2$ reduces the problem to the 2TP problem, i.e."reflects" the negative region $r < 0$ (and zeroes of the w.f.) into the positive region. A more correct approach to solve the problem would be a 4TP quantization condition. Fortunately, the WKB method in the complex plane allows to solve this problem as the 4TP problem.

In the complex plane, the problem has two cuts, between turning points r_1, r_2 and r_3, r_4. To apply residue theory for the phase space integral we need to take into account all zeroes of the w.f. in the complex plane, i.e. the contour C has to include both cuts. The quantization condition (19) in this case takes the form

$$\oint_C \left[p(r,E) + i\frac{\hbar}{2}\frac{p'(r,E)}{p(r,E)}\right] dr \equiv \tag{36}$$
$$\oint_{C_1} \left[p(r,E) + i\frac{\hbar}{2}\frac{p'(r,E)}{p(r,E)}\right] dr + \oint_{C_2} \left[p(r,E) + i\frac{\hbar}{2}\frac{p'(r,E)}{p(r,E)}\right] dr = 2\pi\hbar N,$$

where $p^2(r,E) = 2mE - (m\omega r)^2 - \vec{M}^2/r^2$, and C_1 and C_2 are the contours about the cuts at $r < 0$ and $r > 0$, respectively. The number $N = n_{r<0} + n_{r>0}$, where $n_{r<0}$ and $n_{r>0}$ are the numbers of zeroes of the w.f. at $r < 0$ and $r > 0$, respectively. For the harmonic oscillator, because of symmetricity of the potential we have $n_{r<0} = n_{r>0} = n_r$, i.e. the total number of zeroes is $N = 2n_r$.

Therefore, the quantization condition (36) for the 4TP problem takes the form,

$$\oint_C p(r,E)dr = \oint_{C_1} p(r,E)dr + \oint_{C_2} p(r,E)dr = 2\pi\hbar k\left(n_r + \frac{1}{2}\right), \tag{37}$$

where $k = 2$ is the number of cuts. We can write the 4TP quantization condition in this form because the effective potential is infinite at $r = 0$. In case if the potential is finite in the whole region, the quantization condition will be more complicate [14].

The condition (37) is in agreement with the Maslov's theory. This means that the right-hand side of the equation (37) can be written in the form

$$2\pi\hbar k\left(n_r + \frac{1}{2}\right) = 2\pi\hbar\left(N + \frac{\mu}{4}\right), \tag{38}$$

where $\mu = 2k$ is the Maslov's index, i.e. number of reflections of the w.f. on the walls of the potential.

In the general case of the potential which is infinite between cuts, the $2k$ turning point quantization condition is

$$\oint_C p(z,E)dz = 2\pi\hbar\sum_{i=1}^{k}\left(n + \frac{1}{2}\right)_i \equiv 2\pi\hbar\left(N + \frac{\mu}{4}\right), \tag{39}$$

where $N = kn_i$ is the total number of zeroes of the w.f. on the k cuts. On the real axis, for the $2k$ TP problem, the quantization condition (39) has the form

$$\sum_{i=1}^{k}\int_{x_{1i}}^{x_{2i}}\sqrt{p^2(z,E)}dz=\pi\hbar\left(N+\frac{\mu}{4}\right). \tag{40}$$

Because the harmonic oscillator potential is symmetric, integrals in Eq. (37) are identical, i.e. the quantization condition (37) is equivalent to the 2TP quantization condition (20). The phase-space integral can be easily calculated in the complex plane. For this we have to exclude the singularities at $r=0$ and ∞ outside the contour C. Excluding these infinities we have, for the integral (39) with the isotropic potential, $I=I_0+I_\infty$, where $I_0=-2\pi M$ and integral I_∞ is calculated with the help of the replacement $r=1/z$, $I_\infty=2\pi E/\omega$, i.e. we again obtain the exact result (35) for E_n.

Consider Eq. (35) at $n_r=0$ and $l=0$, i.e. the energy of the ground state. We have $E_0=\omega(\hbar+M_0)$, where $M_0=\hbar/2$ is the contribution of the quantum fluctuations of the angular momentum into the energy of the ground state E_0. The radial quasiclassical eigenfunctions, $\tilde{R}_n^{WKB}(r)$, in the region of the classical motion far from the turning points are written analogously to the above case in the form of a standing wave [see Eq. (33)] .

D. The Hulthén potential $V(r)=-V_0e^{-r/r_0}/(1-e^{-r/r_0})$. The Hulthén potential is of a special interest in atomic and molecular physics. The potential is known as an "insoluble" by the standard WKB method potentials, unless one supplements it with Langer-like corrections. The radial problem for this potential is usually considered at $l=0$. However, in the approach under consideration, the quasiclassical method results in the nonzero centrifugal term at $l=0$ and allows to obtain the analytic result for all l.

The leading-order WKB quantization condition (20) for the Hulthén potential is

$$I=\oint\sqrt{2m\left(E+V_0\frac{e^{-r/r_0}}{1-e^{-r/r_0}}\right)-\frac{\vec{M}^2}{r^2}}dr=2\pi\hbar\left(n_r+\frac{1}{2}\right). \tag{41}$$

In the region $r>0$, this problem has two turning points r_1 and r_2. The phase-space integral (41) is calculated analogously to the above case. Introducing the new variable $\rho=r/r_0$, we calculate the contour integral in the complex plane, where the contour C encloses the classical turning points ρ_1 and ρ_2. Using the method of stereographic projection, we should exclude the infinities at $r=0$ and ∞ outside the contour C. Excluding these infinities we have, for the integral (41), $I=I_0+I_\infty$, where $I_0=-2\pi M$ and I_∞ is calculated with the help of the replacement $z=e^\rho-1$ [5],

$$I=\oint\sqrt{2mr_0^2\left(E+V_0\frac{e^{-\rho}}{1-e^{-\rho}}\right)-\frac{\vec{M}^2}{\rho^2}}d\rho= \tag{42}$$
$$-2\pi M+2\pi r_0\sqrt{-2m}\left[-\sqrt{-E}+\sqrt{-E+V_0}\right].$$

Substituting the integration result into Eq. (41), we immediately get the exact energy spectrum

$$E_n=-\frac{1}{8mr_0^2}\left(\frac{2mV_0r_0^2}{N}-N\right)^2. \tag{43}$$

where $N = (n_r + \frac{1}{2})\hbar + M$ is the principal quantum number. Setting in (43) $M = 0$, we arrive at the energy eigenvalues obtained from known exact solution of the Schrödinger's equation at $l = 0$. However, in our case $M_{min} \equiv M_0 = \hbar/2$ at $l = 0$ and the principal quantum number is $N = (n_r + \frac{1}{2})\hbar + M_0$. As in the previous examples, this apparently shows the contribution of the quantum fluctuations of the angular momentum into the energy of the ground state, E_0.

E. The Morse potential $V(r) = V_0[e^{-2\alpha(r/r_0-1)} - 2\ e^{-\alpha(r/r_0-1)}]$. The Morse potential is usually considered as one-dimensional problem at $l = 0$. In this case the problem has two turning points (note that the left turning point, r_1, is negative) and can be solved exactly. In the general case, for $l > 0$, we have an "insoluble" 4TP problem.

For this potential, let us consider, first, the radial Schrödinger equation (2), which does not contain the centrifugal term at $l = 0$,

$$\left(-i\hbar\frac{d}{dr}\right)^2 U(r) = 2m\left[E - V_0 e^{-2\alpha(r-r_0)/r_0} + 2V_0 e^{-\alpha(r-r_0)/r_0}\right] U(r). \tag{44}$$

The first-order WKB quantization condition (5) appropriate to this equation is

$$\int_{r_1}^{r_2} \sqrt{2m[E - V_0 e^{-2\alpha(r-r_0)/r_0} + 2V_0 e^{-\alpha(r-r_0)/r_0}]}dr = \pi\hbar\left(n_r + \frac{1}{2}\right). \tag{45}$$

Introducing a variable $x = e^{-\alpha(r-r_0)/r_0}$, we reduce the phase-space integral to the well known one. Sequential simple calculations result in the exact energy eigenvalues

$$E_n = -V_0\left[1 - \frac{\alpha\hbar(n_r + \frac{1}{2})}{r_0\sqrt{2mV_0}}\right]^2. \tag{46}$$

Now, let us deal with Eq. (12) for this potential, which contains the non-vanishing centrifugal term, $\hbar^2/4r^2$, at $l = 0$. In this case we have an "insoluble" 4TP problem. In the complex plane, the problem has two cuts ($k = 2$), at $r < 0$ and $r > 0$, therefore, we apply the 4TP quantization condition (37),

$$I = \oint_C \sqrt{2m\left[E - V_0 e^{-2\alpha(r-r_0)/r_0} + 2V_0 e^{-\alpha(r-r_0)/r_0}\right] - \frac{\vec{M}^2}{r^2}}dr = 4\pi\hbar\left(n_r + \frac{1}{2}\right), \tag{47}$$

where the contour C encloses the two cuts, but does not enclose the point $r = 0$. To calculate this integral introduce the variable $\rho = r/r_0$. Using the method of stereographic projection, we should exclude the singularities outside the contour C, i.e. at $r = 0$ and ∞. Excluding these infinities we have, for the integral (47) [5],

$$I = -2\pi M - \frac{2\pi r_0}{\alpha}\left(\sqrt{-2mE} - \sqrt{2mV_0}\right), \tag{48}$$

and for the energy eigenvalues this gives

$$E_n = -V_0\left[1 - \alpha\frac{2\hbar(n_r + \frac{1}{2}) + M}{r_0\sqrt{2mV_0}}\right]^2. \tag{49}$$

Setting in (49) $l = 0$, we obtain,

$$E_n = -V_0 \left[1 - \frac{\alpha[2\hbar(n_r + \frac{1}{2}) + M_0}{r_0\sqrt{2mV_0}} \right]^2 . \tag{50}$$

Equation (50) for E_n is different from the expression (46) obtained from solution of Eq. (2) for the Morse potential at $l = 0$. This difference is caused by the nonzero centrifugal term $\hbar^2/4r^2$ in the radial equation (12) at $l = 0$. Thus we obtain two results for the Morse potential by the WKB method: the known exact eigenvalues (46) obtained from solution of Eq. (2) at $l = 0$ and another result (49) obtained from solution of Eq. (12) for all l.

F. The potential $V(r) = kr + \frac{1}{2}\omega^2 r^2$. This linear plus isotropic potential is one of the interest in particle physics. The potential has four turning points and can not be reduced to a hypergeometric function by a suitable transformation. This multi-turning-point problem is "insoluble", also, by the standard WKB method. However, the WKB method in the complex plane allows easily to solve this 4TP problem [see, for instance, Refs. [22, 23]].

The problem has two cuts ($k = 2$) in the complex plane between turning points r_1, r_2 and r_3, r_4. Quantization condition (39), for this problem, is

$$I = \oint_C \sqrt{2mE - 2mkr - (m\omega r)^2 - \frac{\vec{M}^2}{r^2}}dr = 4\pi\hbar \left(n_r + \frac{1}{2} \right), \tag{51}$$

where the contour C includes both cuts, but includes no the point $r = 0$. To calculate the integral (51) we exclude the infinities at $r = 0$ and ∞ outside the contour C. Excluding these infinities we have, for the integral (51),

$$I = 2\pi \left[\frac{E}{\omega} + \frac{1}{2m\omega} \left(\frac{k}{\omega} \right)^2 - M \right] = 4\pi\hbar \left(n_r + \frac{1}{2} \right), \tag{52}$$

or, for the energy eigenvalues, this gives

$$E_n = \omega \left[2\hbar \left(n_r + \frac{1}{2} \right) + M \right] - \frac{1}{2m} \left(\frac{k}{\omega} \right)^2 . \tag{53}$$

Energy eigenvalues (53) are similar to the harmonic oscillator ones but shifted by the constant value $-\frac{1}{2m}(k/\omega)^2$. Putting in Eq. (53) $k = 0$, we arrive to the eigenvalues (35) for the isotropic oscillator.

Analogously one can obtain energy eigenvalues for other spherically symmetric potentials. The standard leading-order WKB approximation appropriate to the wave equation (12) yields the exact energy eigenvalues for known solvable potentials and "insoluble" ones with more than two turning points. This is possible because the centrifugal term of the required form, $(l + \frac{1}{2})^2\hbar^2/r^2$, has obtained in a natural way from solution of the angular equation (13) with the use of the same WKB method; this term is the same for all central-field potentials.

5. Conclusion

Conventional approach to solve the Schrödinger's equation is to reduce the original equation to a hypergeometric form or some special function by a suitable transformation. In each and every case, one needs to find, first, a special transformation for the wave function and its arguments to reduce the original equation to some known equation. There is another way to solve the Schrödinger's equation which is simple, general for all types of problems in quantum mechanics, and a very efficient to solve not only two- but multi-turning point problems.

Almost together with quantum mechanics an appropriate method to solve the wave equation has been developed known mainly as the WKB approximation. This method is general for all types of problems in quantum mechanics, simple from the physical point of view, and its correct application results in the exact energy eigenvalues for *all* solvable potentials.

In spite of long history no any strict rules concerning the application of the WKB method to multi-dimensional problems in quantum mechanics have been formulated. Meanwhile, this topic is closely related to the problem of exactness of the WKB method. The exactness of the method has proven in the literature for many potentials with the help of specially developed techniques, or improvements, or modifications of the quasiclassical method on the real axis and in the complex plane. In this work we have fulfilled the quasiclassical analysis of the three-dimensional Schrödinger's equation. The original equation has been reduced to the form of the classic Hamilton-Jacobi equation without first derivatives. Separation of the equation has been performed with the help of the correspondence principle between classic and quantum-mechanical quantities. As a result of the separation, we have obtained the system of reduced second-order differential equations. Each of these equations has the correct quantum-mechanical form, $\hat{p}_q^2\psi(q) = p^2(q)\psi(q)$, and solved by the WKB method. We have stressed that the squared generalized moments, $p^2(q)$, obtained after separation should coincide with the corresponding classic moments. This means that the problem under consideration should correspond to a concrete classic problem.

We have shown that the Langer replacement $l(l+1) \to (l+\frac{1}{2})^2$ needed to reproduce the exact energy spectrum for the spherically symmetric potentials by the WKB method requires the modification of the squared angular momentum in the quasiclassical region. The squared angular momentum eigenvalues, $\vec{M}^2 = (l+\frac{1}{2})^2\hbar^2$, have obtained in our approach from solution of the angular wave equation in the framework of the same quasiclassical method. As a result, the centrifugal term has the form $(l+\frac{1}{2})^2\hbar^2/r^2$ for *any* spherically symmetric potential $V(r)$.

The quasiclassical solution contains a more detail information in comparison with known exact solution. One of consequences of the WKB solution of the Schrödinger's equation is the existence of a nontrivial angular eigenfunction of the type of a standing half-wave for the angular quantum number $l = 0$. This solution has treated as one which describes the quantum fluctuations of the angular momentum with the eigenvalue $M_0 = \hbar/2$. We have shown that the quantum fluctuations of the angular momentum contribute to the energy of the ground state, E_0.

To demonstrate efficiency of the quasiclassical method, we have solved the three-

dimensional Schrödinger's equation for some central-field potentials. The quasiclassical method successfully reproduces the exact energy spectrum not only for solvable spherically symmetric potentials but, also, for "insoluble" potentials with more than two turning points. The quasiclassical eigenfunctions for the discrete spectrum have written in elementary functions in the form of a standing wave.

The remarkable features of the quasiclassical method incline us to treat the leading-order WKB approximation as a special (asymptotic) exact method to solve the Schrödinger equation. In the quasiclassical approach we use the same technique for all types of problems. The same simple rules formulated for two-turning problems work for many turning point problems, as well. In this sense, the quasiclassical method is a more general in comparison with traditional one with the use of techniques of the special functions.

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